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SPACE AND TIME DEPENDENT EIGENVALUE PROBLEM IN NEUTRON THERMALIZATION

by H. TAKAHASHI

1962

JOINT NUCLEAR RESEARCH CENTER
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Reactor Physics Department

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Joint Nuclear Research Center
Ispra Establishment (Italy) - Reactor Physics Department
Brussels, September 1962 - pages 25 - fig. 4.

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The results obtained for beryllium and graphite are respectively 3.36 and 2.4 times larger than those obtained by the Nelkin theory.

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SPACE AND TIME DEPENDENT EIGENVALUE PROBLEM IN NEUTRON THERMALIZATION *

SUMMARY

The matrix elements of the neutron scattering kernel for a free-gas and crystalline material expanded in terms of Laguerre polynomials of energy, weighted by a Maxwellian distribution, are obtained by a generating function for the Laguerre polynomial. The eigenvalue problems in a spatial and time dependent neutron thermalization are solved by using the obtained matrix element. For the spatial problem first order Laguerre polynomials are used. Half order Laguerre polynomials are used for the time dependent problem, because they diagonalize respectively the spatial and the time dependent term.

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1 — INTRODUCTION

The time dependent problem using a pulsed neutron, and the space dependent problem have been considered by many authors (1 ~ 15) for the study of neutron thermalization. Experimental data (13, 14, 15) have been accumulated and theories also have been developed by using the variational method (3, 4) and the expansion method of flux in terms of orthogonal polynomials (5,12). In the variational method, if simple trial functions are used, simple analytical formulations are obtained. From these formulations we can get the physical meaning of the phenomena avoiding a tedious numerical calculation. Sometimes, however, the numerical results obtained from variational approach are not very accurate. When an accurate numerical value is needed, it is better to adopt the expansion method. Although this method has been used for the neutron thermalization problem, only the low order expansion (5,9) has been considered except the case of heavy gas model (6 ~ 7, 10 ~ 12) and of free gas with mass 1 (8). In the heavy gas model, the matrix of the scattering kernel is diagonalized in terms of first order Laguerre polynomials.

In this paper, the matrix elements of the scattering kernel for free-gas and crystalline material expanded in terms of the Laguerre polynomial, which is weighed by the Maxwellian distribution, are obtained by using the generating function of Laguerre polynomials. In the case of space dependent problem with energy independent diffusion coefficient, first order Laguerre polynomials, diagonalizing the diffusion term, are used to expand the flux, and half order Laguerre polynomials are used for the time dependent problem,

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where the term differentiated by time with a $1/\sqrt{E}$ energy dependence is diagonalized. In Laguerre polynomials, the generating function of the scattering kernel in the space dependent problem is simply related to the one of the time dependent problem. The generating function for the crystalline material is calculated by the Plazeck's mass expansion method, the phonon expansion method (17, 18) and two frequency dividing methods (21) which have been used for a calculation of total cross section and differential cross section of neutron scattering.

The time and space dependent eigenvalues and eigenfunctions for free-gas, Debye crystalline and graphite are calculated. A convergence of spatial eigenvalues obtained by increasing the dimension of matrix is very good. However, the convergence of time dependent eigenvalues is rather slow. The diffusion cooling coefficient obtained from the decay constant of pulsed neutrons in a small assembly has been calculated from the thermalization power M_2. The Nelkin's formulation for the diffusion cooling corresponds to the formulation in which only the first two terms of the Laguerre expansion are kept. The Nelkin's formulation gives a comparatively good numerical value in the case of free gas model. However, in the case of crystalline materials like beryllium and graphite, the accurate results are: in beryllium a 3.3 times larger value than the Nelkin's results, in graphite a 2.4 times larger value than the results from Nelkin's formula.

2 — GENERAL FORMULATION

The Boltzmann equation for the time and spatial dependent angular flux $f(\vec{r}, E, \vec{\Omega}, t)$ is (16):

$$\frac{1}{v}\frac{\partial f(\vec{r}, E, \vec{\Omega}, t)}{\partial t} = -\vec{\Omega}\cdot\operatorname{grad} f(\vec{r}, E, \vec{\Omega}, t) + \int\int dE'\, d\Omega'\, f(\vec{r}, E', \vec{\Omega}', t)\Sigma_s(\vec{r}, E' \to E, \vec{\Omega}' - \vec{\Omega}) - \Sigma(\vec{r}, E, \vec{\Omega}) f(\vec{r}, E, \vec{\Omega}, t) + S(\vec{r}, E, \vec{\Omega}) \tag{1}$$

Since we are interested in the eigenvalue problem, we shall take the source term $S(\vec{r}, E, \vec{\Omega})$ to be zero. In the diffusion approximation equation (1) takes the form:

$$\frac{1}{v}\frac{\partial \Phi(\vec{r}, E, t)}{\partial t} - D(E)\,\nabla^2\Phi(\vec{r}, E, t) + \Sigma_a\Phi(\vec{r}, E, t) - \int_0^\infty \Phi(\vec{r}, E, t)\Sigma_s(E' \to E)dE' + \Sigma_s(E)\Phi(\vec{r}, E, t) = 0 \tag{2}$$

where

$$\Phi(\vec{r}, E, t) = \int d\Omega\, f(\vec{r}, E, \Omega, t)$$

By making a Laplace transformation for the time variation, and for the spatial variation, expanding the flux in terms of the eigenfunction of the equation:

$$\nabla^2 \chi_l(r) + B_l^2 \chi_l(r) = 0$$

where B^2 is the buckling corresponding to the 1st harmonic, the time variation and the spatial variation can be separated from the equation (2), and the problem reduces to a following time and space independent equation, in which the time constant λ or B^2 appears as an eigenvalue.

$$-\frac{\lambda}{v}\Phi(E) + D(E)\,B^2\,\Phi(E) + \Sigma_a(E)\Phi(E) + \Sigma_s(E)\Phi(E) - \int_0^\infty \Phi(E')\Sigma_s(E' \to E)\,dE' = 0 \qquad (3)$$

In order to simplify matters, we shall consider the spatial eigenvalue problem and time eigenvalue problem separately. Since the moderator material generally shows the $1/v$ absorption cross section, it is suitable to include the absorption cross section terms in the time eigenvalue problem, and to treat the spatial eigenvalue problem in the non absorbing medium.

2.1 — Space dependent problem

Let us first consider the spatial eigenvalue problem in the case of energy independent diffusion coefficient:

$$DB^2\,\Phi(E) + \Sigma_s(E)\Phi(E) - \int_0^\infty \Phi(E')\Sigma_s(E' \to E)\,dE' = 0 \qquad (4)$$

We assume that $\Phi(E)$ can be expressed as:

$$\Phi(E) = \sum_{i=0}^{\infty} \frac{1}{\sqrt{i+1}} L_i^{(1)}\left(\frac{E}{T}\right) \frac{E}{T^2}\, e^{-\frac{E}{T}}\, a_i \qquad (5)$$

where $L_i^{(1)}(x)$ is the generalized Laguerre polynomial of order unity and degree of i and the Laguerre polynomial of order α, $L_i^{(\alpha)}(x)$ has the following generating function:

$$\frac{e^{-X\frac{P}{1-P}}}{(1-P)^{\alpha+1}} = \sum_{i=0}^{\infty} P^i L_i^{(\alpha)}(X) \quad (*) \qquad (6)$$

(*) In this paper, the Laguerre polynomial with the orthonormality eq (7) has been used instead of the Laguerre polynominal defined in the text book (Method of Theoretical Physics, Morse & Freshback). The reason is that this Laguerre polynominal is more convenient than the others for numerical calculation using the calculating machine.

The polynomial has the following orthonormality:

$$\int_0^\infty L_i^{(\alpha)}(x)\, L_j^{(\alpha)}(x)\, x\ \mathrm{e}^{-x}\, dx = \delta_{ij}\frac{\Gamma(i+1+\alpha)}{\Gamma(i+1)} \tag{7}$$

Substituting (5) into (4) and multiplying the resulting equation by $\frac{1}{\sqrt{(j+1)}} L_j^{(1)}\left(\frac{E}{T}\right)$ and integrating over E, we get

$$DB^2\,\delta_{ij}\,a_i - S_{ij}\,a_i = 0 \tag{8}$$

where

$$S_{ij} = \frac{1}{\sqrt{(i+1)(j+1)}}\left[\int_0^\infty\int_0^\infty dE'\,dE\,\Sigma_s(E'\to E)L_i^{(1)}\left(\frac{E'}{T}\right)L_j^{(1)}\left(\frac{E}{T}\right)\frac{E'}{T^2}\ \mathrm{e}^{-\frac{E'}{T}}\right.$$

$$\left. -\int_0^\infty\int_0^\infty dE'\,dE\,\Sigma_s(E'\to E)L_i^{(1)}\left(\frac{E'}{T}\right)L_j^{(1)}\left(\frac{E'}{T}\right)\frac{E'}{T^2}\ \mathrm{e}^{-\frac{E'}{T}}\right] \tag{9}$$

It is well known that the heavy gas model has been frequently used in the neutron thermalization problem because the matrix (S_{ij}) is diagonalized simultaneously with energy independent spatial term DB^2 by this Laguerre polynomial.

Next, we shall consider the evaluation of the matrix (S_{ij}).

In the incoherent approximation, the formula for the differential cross section in the neutron scattering by the crystalline material can be written in the form:

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k}{k'}\cdot\frac{\Sigma_B}{8\pi^2}\int_{-\infty}^{\infty}\exp\left[-\kappa^2(M(0)-M(t))\right]\exp(i(\omega-\omega')t)\,dt \tag{10}$$

$\omega = E/\hbar$, where E is the energy of the scattered neutron, Ω is the solid angle, k' and k are the wave vectors of the incoming and scattered neutron and $\vec{\kappa^2} = k'-k$, Σ_B is the bounded cross section, and $M(t)$ is related to the frequency spectrum $f(\omega)$ as follows:

$$\begin{aligned} M(t) &= \frac{\hbar}{2M}\int_0^{\omega_m}\left[\coth(\beta\omega)\cos(\omega t) + i\sin\omega t\right]\ \frac{f(\omega)}{\omega}\,d\omega \\ &= \frac{\hbar}{2M}\gamma(t) \end{aligned} \tag{11}$$

where M is the mass of atom, m the neutron mass, and $\beta = \frac{\hbar}{2T}$.

In the calculation of matrix element (S_{ij}), we use the generating function of (6) for the Laguerre polynomial. Let us consider the first terms $S_{ij}^{(1)}$ in the matrix S_{ij} of eq (9), which are obtained as the coefficient of $\sqrt{(i+1)(j+1)}P^iI^j$ in the following generating function:

$$S^{(1)} = \int\int\int_0^\infty \frac{d^2\sigma}{d\Omega d\omega}(1-P)^{-2}(1-I)^{-2}\exp\left(-\frac{E'}{T}\left(\frac{P}{1-P}\right)\right)$$

$$\cdot \exp\left(-\frac{E}{T}\left(\frac{l}{1-l}\right)\right)\frac{E'}{T^2}\, e^{-\frac{E'}{T}}\, dE'\, d\Omega d\omega \tag{12}$$

Substituting eq (10) to eq (12), we get:

$$S^{(1)} = \int\int\int_{-\infty}^{\infty} \frac{\hbar}{mk'}\frac{\Sigma_B}{8\pi^2}\exp\left[-\kappa^2(M(0)-M(t))\right]\exp(i(\omega-\omega')t)$$

$$\cdot (1-P)^{-2}(1-l)^{-2}\exp\left(-\frac{E'}{T}\left(\frac{P}{1-P}+1\right)\right)\exp\left(-\frac{E}{T}\left(\frac{l}{1-l}\right)\right)\frac{E'}{T^2}\,dt\,dE'\,d\vec{\kappa^3} \tag{13}$$

By substituting the following relation into eq (13):

$$\hbar\omega = \hbar\omega' - 2\sqrt{\hbar\omega'}\frac{\hbar\kappa}{\sqrt{2m}}\cos\theta + \frac{\hbar^2\kappa^2}{2m} \tag{14}$$

we get:

$$S^{(1)} = \frac{\Sigma_B}{8\pi^2}(1-P)^{-2}(1-l)^{-2}\int_{-\infty}^{\infty}\int\int\frac{\hbar}{m}\exp(-\hbar\omega'(I+J))\frac{E'}{k'}$$

$$\exp\left(-\frac{\hbar\kappa^2}{2m}(it-\hbar J)-\frac{2m}{\hbar}(M(0)-M(t))\right)\exp\left(-2\sqrt{\hbar\omega}\frac{\kappa}{\sqrt{2m}}(it-\hbar J)\cos\theta\right)d\vec{\kappa^3}\,dE'\,dt$$

$$= \frac{\Sigma_B}{8}\frac{\hbar^2}{T^2}(1-P)^{-2}(1-l)^{-2}\int_{-\infty}^{\infty}\frac{dt}{\left[(t-i\hbar I)(t+i\hbar J)+(I+J)2m(M(0)-M(t))\right]^{3/2}} \tag{15}$$

$$\text{where } I = \left(\frac{P}{1-P}+1\right)\frac{1}{T} \text{ and } J = \left(\frac{l}{1-l}\right)\frac{1}{T} \tag{16}$$

The generating function for the second term of eq (9) $S^{(2)}$ is obtained by the same way with $S^{(1)}$ as follows:

$$S^{(2)} = \int\int\int_{0}^{\infty}\frac{d^2\sigma}{d\Omega d\omega}(1-P)^{-2}(1-l)^{-2}\exp\left(-\frac{E'}{T}\left(1+\frac{P}{1-P}+\frac{l}{1-l}\right)\right)dE'\,d\Omega\,d\omega$$

$$= \frac{\Sigma_B}{8}\frac{\hbar^2}{T^2}(1-P)^{-2}(1-l)^{-2}\int_{-\infty}^{\infty}\frac{dt}{\left[t(t-i\hbar(I+J))+(I+J)2m(M(0)-M(t))\right]^{3/2}} \tag{17}$$

The generating function for matrix S is:

$$S = S^{(1)} - S^{(2)} \tag{18}$$

2.1.1 — *Free-gas case*

The effects of crystalline material are included in the term of $[M(0)-M(t)]$. If we take the upper limit ω_m (Debye frequency) of frequency function $f(\omega)$ to be zero, that is, the atomic force between the composed atom becomes zero, this expression becomes the one of the free gas model. In this case, the function $[M(0)-M(t)]$ is expressed in the following form:

$$M(0)-M(t)=-\frac{\hbar}{2M}\left(it-\frac{T}{\hbar}t^2\right) \tag{19}$$

Substituting eq (18) into eq (15),

$$S^{(1)}=\Sigma_B\frac{\left(1+\frac{m}{M}\left(1+\frac{P}{1-P}+\frac{l}{1-l}\right)\right)^{1/2}}{\left[(1-Pl)^2\left(1+\frac{m}{M}\right)^2+4Pl(1-Pl)\frac{m}{M}\right]} \tag{20}$$

Similarly, we get:

$$S^{(2)}=\Sigma_B\frac{\left(1+\frac{m}{M}\left(1+\frac{P}{1-P}+\frac{l}{1-l}\right)\right)^{1/2}}{(1-Pl)^2\left(1+\frac{m}{M}\right)^2} \tag{21}$$

and

$$S=-\frac{4\Sigma_B\frac{m}{M}}{\left(1+\frac{m}{M}\right)^{1/2}}\;\frac{Pl}{(1-Pl)^2}\;\frac{\left[1+\frac{\frac{m}{M}}{1+\frac{m}{M}}\left(\frac{P}{1-P}+\frac{l}{1-l}\right)\right]^{1/2}}{\left[1-\frac{\left(1-\frac{m}{M}\right)^2}{\left(1+\frac{m}{M}\right)^2}Pl\right]} \tag{22}$$

In the case of heavy gas model, by putting $\frac{m}{M}\to 0$, we get:

$$S_{Heavy}=-4\,\Sigma_{free}\frac{m}{M}\frac{Pl}{(1-Pl)^3} \tag{23}$$

We can easily find out from eq (23) that the matrix in the heavy gas model is diagonalized.

2.1.2 — *Crystalline material*

For the case of the crystalline material, the Plazeck's mass expansion method, the phonon expansion method, and the two frequency dividing methods, which have been used for the calculation of total cross section and differential cross section, are applied to the calculation of the integrations in eq (15) and (17).

In the mass expansion method, the integrant in eq (15) is expanded by the power series of $\left(\frac{m}{M}\right)$ as follows:

$$S^{(1)}=\frac{\Sigma_B}{8}\frac{\hbar^2}{T^2}(1-P)^{-2}(1-l)^{-2}$$

$$\cdot\sum_{q=0}^{\infty}(-1)^q\frac{\Gamma\left(\frac{3}{2}+q\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(q+1)}\left(\frac{m}{M}\right)^q\int_{-\infty}^{\infty}\frac{[(I+J)\hbar\Gamma(t)]^q}{[(t-i\hbar I)(t+i\hbar J)]^{3/2+q}}dt \tag{24}$$

where

$$\Gamma(t)^q=[\gamma(0)-\gamma(t)]^q$$

$$=\gamma(0)^q\sum_{n=0}^{q}\frac{\Gamma(q+1)}{\Gamma(q-n+1)\Gamma(n+1)}\int_{-\infty}^{\infty}G_n(\omega)\,e^{-i\omega t}\,d\omega \tag{25}$$

where $G_o(\omega)=\delta(\omega)$

$$G_n(\omega)=\frac{(-1)^n}{\gamma(0)^n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\frac{f(\omega-\omega_1)}{(\omega-\omega_1)}\,\frac{\coth\beta(\omega-\omega_1)-1}{2}$$

$$\cdot\frac{f(\omega_1-\omega_2)}{(\omega_1-\omega_2)}\,\frac{\coth\beta(\omega_1-\omega_2)-1}{2}\cdots\frac{f(\omega_n)}{\omega_n}\,\frac{\coth\beta\omega_n-1}{2}d\omega_1\cdots d\omega_n \tag{26}$$

and using the formulation

$$\int_{-\infty}^{\infty}\frac{e^{-i\omega t}}{[(t-i\hbar I)(t+i\hbar J)]^{3/2+q}}dt$$

$$=2\,e^{\frac{I-J}{2}\hbar\omega}\left(\frac{|\omega|}{(I+J)\hbar}\right)^{q+1}\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(q+\frac{3}{2}\right)}K_{q+1}\left(\frac{I+J}{2}\hbar|\omega|\right) \tag{27}$$

where $K_q(x)$ is the modified Hankel function.

We get:

$$S^{(1)}=\frac{\Sigma_B}{2}\frac{\hbar^2}{T^2}(1-P)^{-2}(1-l)^{-2}\left\{\sum_{q=0}^{\infty}\left(-\frac{m\hbar}{M}\gamma(0)(I+J)\right)^q\right.$$

$$\left.\cdot\sum_{n=0}^{q}\frac{1}{\Gamma(q-n+1)\Gamma(n+1)}\int_{-\infty}^{\infty}G_n(\omega)\left(\frac{|\omega|}{(I+J)\hbar}\right)^{q+1}K_{q+1}\left(\frac{I+J}{2}\hbar|\omega|\right)e^{\frac{I-J}{2}\hbar\omega}d\omega\right\} \tag{28}$$

Similarly:

$$S^{(2)}=\frac{\Sigma_B}{2}\frac{\hbar^2}{T^2}(1-P)^{-2}(1-l)^{-2}\left\{\sum_{q=0}^{\infty}\left(-\frac{m\hbar}{M}\gamma(0)(I+J)\right)^q\right.$$

$$\left.\cdot\sum_{n=0}^{q}\frac{1}{\Gamma(q-n+1)\Gamma(n+1)}\int_{-\infty}^{\infty}G_n(\omega)\left(\frac{|\omega|}{(I+J)\hbar}\right)^{q+1}K_{q+1}\left(\frac{I+J}{2}\hbar|\omega|\right)e^{\frac{I+J}{2}\hbar\omega}d\omega\right\} \tag{29}$$

From eq (28) and eq (29):

$$S=-2\frac{\Sigma_B}{(1-Pl)(1-P)(1-l)}\left\{\sum_{q=1}^{\infty}\left(-\frac{m}{M}Z\right)^q\cdot\sum_{n=1}^{q}\frac{1}{\Gamma(q-n+1)\Gamma(n+1)}\right.$$

$$\left.\int_0^{\infty}\sinh\left(\frac{P}{1-P}\zeta\right)\sinh\left(\frac{l}{1-l}\zeta\right)G'_n(\zeta)\zeta^{q+1}K_{q+1}\left(\left(1+\frac{P}{1-P}+\frac{l}{1-l}\right)\zeta\right)d\omega\right\} \tag{30}$$

where

$$G'_n(\zeta)=\left(\frac{-1}{Z}\right)^n\int_0^{\infty}\cdots\int_0^{\infty}\prod_{i=1}^{n-1}\left[\frac{f(\omega_{i-1}-\omega_i)}{(\zeta_{i-1}-\zeta_i)}\frac{1}{2\sinh(\zeta_{i-1}-\zeta_i)}\right.$$

$$\left.+\frac{f(\omega_{i-1}+\omega_i)}{(\zeta_{i-1}+\zeta_i)}\frac{1}{2\sinh(\zeta_{i-1}+\zeta_i)}\right]\frac{f(\omega_n)}{\zeta_n\sinh\zeta_n}\,d\omega_1\cdots d\omega_n \tag{31}$$

$$Z=\frac{\gamma(0)}{\beta},\quad \zeta_n=\beta\omega_n \text{ and } \zeta_o=\zeta.$$

In phonon expansion method, the integrant in eq. (17) is expanded by:

$$\sum_{q=0}^{\infty}\frac{\Gamma\left(\frac{3}{2}+q\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(q+1)}\left(\frac{m}{M}\right)^q\int_{-\infty}^{\infty}\frac{[(I+J)\hbar\gamma(t)]^q}{[(t-i\hbar I)(t+i\hbar J)+\frac{m}{M}\hbar\gamma(0)(I+J)]^{3/2+q}}dt \tag{32}$$

By similar calculation as the mass expansion method, we get:

$$S=\frac{-2\Sigma_B}{(1-Pl)(1-P)(1-l)}\sum_{q=0}^{\infty}\left(\frac{m}{M}\right)^q\frac{1}{\Gamma(q+1)}$$

$$\cdot\int_0^{\infty}\sinh\left(\frac{P}{1-P}\zeta\right)\sinh\left(\frac{l}{1-l}\zeta\right)G'_q(\zeta)\frac{\zeta^{q+1}K_{q+1}\left(\gamma_1\frac{1-Pl}{(1-P)(1-l)}\zeta\right)}{\gamma_1{}^{q+1}}d\omega \tag{33}$$

where

$$\gamma_1=\sqrt{1+4\frac{m}{M}\frac{\gamma(0)}{\hbar T}\frac{(1-P)(1-l)}{(1-Pl)}}$$

In the case that mass M approaches to one, the convergence of series in the eqs. (32) and (33) becomes slow. In order to calculate the differential cross section, the author developed the two frequency dividing model (22) in which the frequency function is divided in two parts in such a way that the high energy approximation is applicable to the low energy frequency and the phonon or mass expansion method is applicable to the other part with high frequency. By using this model, we can improve the convergence of the series in the phonon or mass expansions. This means that the function $[M(0)-M(t)]$ is divided into the following two integrals by the cut frequency ω_c

$$[M(0)-M(t)]=\frac{\hbar}{2M}\left\{\int_0^{\omega_c}\coth\beta\omega\,\frac{f(\omega)}{\omega}\,d\omega-\int_0^{\omega_c}[\coth\beta\omega\cos\omega t+i\sin\omega t]\,\frac{f(\omega)}{\omega}\,d\omega\right.$$

$$\left.+\int_{\omega_c}^{\omega_m}\coth\beta\omega\,\frac{f(\omega)}{\omega}\,d\omega-\int_{\omega_c}^{\omega_m}[\coth\beta\omega\cos\omega t+i\sin\omega t]\,\frac{f(\omega)}{\omega}\,d\omega\right\} \tag{34}$$

The integration in the low energy frequency part from 0 to ω_c is expanded by power series of t. However, if the ω_c is not small enough compared with the temperature, the neglect of higher term of t^n spoils the energy balance. If we assume that the low energy frequency part is located in the very small energy compared with the temperature T, the integration of $M(0)-M(t)$ over the low energy region is expressed by:

$$-\frac{\hbar}{2M_e}\left(it-\frac{Tt^2}{\hbar}\right) \tag{35}$$

where M_e is the effective mass for the low frequency part, and is defined as:

$$M_e=M\left(1-\int_{\omega_c}^{\omega_m}f(\omega)d\omega\right) \tag{36}$$

By this approximation and applying the mass expansion method to the high frequency part, the generating function S is expressed by:

$$S=\frac{\Sigma_B}{2}\frac{T^2}{\hbar^2}(1-P)^{-2}(1-l)^{-2}\sum_{q=0}^{\infty}\frac{\left(-\frac{m}{M}\hbar\gamma(0)(I+J)\right)^q}{\left[1+\frac{m_e}{M}(I+J)T\right]^{3/2+q}}$$

$$\sum_{n=0}^{q}\frac{1}{\Gamma(q-n+1)\Gamma(n+1)}\int_{-\omega_m}^{''\omega_m}G_n''(\omega)\left\{\left(\frac{|\omega|}{(I'+J')\hbar}\right)^{q+1}K_{q+1}\left(\frac{I'+J'}{2}\hbar|\omega|\right)e^{\frac{I'-J'}{2}\hbar\omega}\right.$$

$$\left.-\left(\frac{|\omega|}{(I''+J'')\hbar}\right)^{q+1}K_{q+1}\left(\frac{I''+J''}{2}\hbar|\omega|\right)e^{\frac{I''+J''}{2}\hbar\omega}\right\}d\omega \tag{37}$$

where the signs ($''$) on the integration sign and $G_n(\omega)$ means that the integration in the expression is done only over the high energy frequency part, where

$$\begin{matrix}I'\\-J'\end{matrix}=\frac{-\left[(J-I)-\frac{m_e}{M}(I+J)\right]\mp\sqrt{\left((J-I)-\frac{m_e}{M}(I+J)\right)^2+4\left(1+\frac{m_e}{M}T(I+J)\right)IJ}}{2\left[1+\frac{m_e}{M}T(I+J)\right]}$$

$$\begin{matrix}I''\\-J''\end{matrix}=\frac{\left[(I+J)\left(1+\frac{m_e}{M}\right)\right]\pm\sqrt{(I+J)^2\left(1+\frac{m_e}{M}\right)^2+4\left(1+\frac{m_e}{M}T(I+J)\right)IJ}}{2\left[1+\frac{m_e}{M}T(I+J)\right]} \tag{38}$$

2.2 — Time dependent problem

The method for the space dependent problem in the last section can easily be extended to the case of time dependent problem. The time dependent equation, in the medium with the $1/v$ absorption is expressed by:

$$-\frac{\lambda}{v}\Phi(E)+\frac{\Gamma}{v}\Phi(E)-\int_0^\infty \Phi(E')\Sigma_s(E'\to E)dE' + \Sigma_s(E)\Phi(E)=0 \tag{39}$$

This equation is easily solved by expanding the terms $-\frac{\lambda}{v}\Phi(E)$ and $\frac{\Gamma}{v}\Phi(E)$ in terms of the Laguerre polynomial of first order energy (from now on, we will include the absorption term $\frac{\Gamma}{v}$ into decay term $\frac{-\lambda}{v}$). But, in the following eigenvalue problem

$$A\,\Psi=\lambda\,B\,\Psi$$

since the large number of calculation codes have been developed for the case that matrix B is diagonalized, it is more convenient to use the other orthogonal set diagonalizing the term which is proportional to $1/v$.

We assume that $\Phi(E)$ can be expressed as:

$$\Phi(E)=\sum_{i=0}^{\infty}\sqrt{\frac{\Gamma(i+1)}{\Gamma\left(i+\frac{3}{2}\right)}}\,L_i^{(1/2)}\left(\frac{E}{T}\right)\frac{E}{T^2}\,e^{-E/T}a_i \tag{40}$$

Substituting eq. (40) into eq. (39) and multiplying the resulting equation by

$$\sqrt{\frac{\Gamma(j+1)}{\Gamma\left(j+\frac{3}{2}\right)}}\,L_j^{(1/2)}\left(\frac{E}{T}\right)$$

and integrating over E, we get:

$$\left[\lambda\,\delta_{ij}-v_0\,S_{ij}^T\right]\,a_i=0 \tag{41}$$

where $v_0=\sqrt{2mT}$

$$S_{ij}^T=\sqrt{\frac{\Gamma(i+1)\Gamma(j+1)}{\Gamma\left(i+\frac{3}{2}\right)\Gamma\left(j+\frac{3}{2}\right)}}\left[\int_0^\infty\int_0^\infty dE'dE\,\Sigma_s(E'\to E)L_i^{(1/2)}\left(\frac{E'}{T}\right)L_j^{(1/2)}\left(\frac{E}{T}\right)\frac{E'}{T^2}e^{-\frac{E'}{T}}\right.$$
$$\left.-\int_0^\infty\int_0^\infty dE'dE\,\Sigma_s(E'\to E)L_i^{(1/2)}\left(\frac{E'}{T}\right)L_j^{(1/2)}\left(\frac{E'}{T}\right)\frac{E'}{T^2}e^{-\frac{E'}{T}}\right] \tag{42}$$

Since the Laguerre polynomial of half order $L_i^{(1/2)}(x)$ has the generating function of eq. (6), the matrix elements S_{ij}^T in eq. (42) are obtained as the coefficient of

$$\sqrt{\frac{\Gamma\left(i+\frac{3}{2}\right)\Gamma\left(j+\frac{3}{2}\right)}{\Gamma(i+1)\Gamma(j+1)}}\,P^i l^j$$

in the following generating function S^T

$$S^T = \sqrt{(1-P)(1-l)}\,S \tag{43}$$

where S is the generating function of the space dependent problem in eq. (18).

Furthermore, if the diffusion coefficient or the absorption cross section is proportional to E^a, the generating function S^a of the matrix for scattering kernel, where the flux is expanded in terms of Laguerre polynomial diagonalizing the diffusion term or the absorption term, is composed from the S in eq. (18) as follows:

$$S^a = [\,(1-P)(1-l)\,]^{-a} S \tag{44}$$

3 — NUMERICAL RESULTS

Since much more works have been studied for the time dependent problem than for the space dependent problem, we will consider mainly the time dependent problem as the application of the above described theory.

The decay constant λ of pulsed neutrons in a small assembly is expressed by: (1 ~ 3)

$$\lambda = (\Sigma_a v) + D_o B^2 - C B^4 \tag{45}$$

where B is the buckling of the assembly, D_o is the diffusion coefficient, Dv averaged over the Maxwellian distribution, and C is the diffusion cooling coefficient.

In the case of an energy independent diffusion coefficient, Nelkin (3) found:

$$C = \frac{\sqrt{\pi}}{4}\,\frac{D_o^2}{v_o M_2} = \frac{D_o^2}{6\,\lambda_{M2}} \tag{46}$$

where M_2 is the thermalization power and is defined as:

$$M_2 = \frac{1}{T^4}\int_0^\infty dE' \int_0^\infty dE\,\Sigma(E' \to E)(E'-E)^2 E'\ e^{-\frac{E'}{T}} \tag{47}$$

and it is related to the matrix element S_{11} and S_{11}^T as follows:

$$M_2 = 4\,S_{11} = \frac{3\sqrt{\pi}\,S_{11}^T}{2} \tag{48}$$

This diffusion cooling coefficient (12) is expressed more exactly by:

$$C = \sum_{m=1}^{\infty} \frac{\left[\int_0^{\infty} \Phi_m^T(E)\,\Phi_o^T(E)\frac{1}{E}\,e^{+\frac{E}{T}}\,dE\right]^2 D^2}{\lambda_m} = \frac{D_o^2}{6\,\overline{\lambda}_1} \tag{49}$$

where λ_m, Φ_m^T, the mth eigenvalue and eigenfunction of time dependent equation (39). Since the term of $m = 1$ contributes mainly in many cases and the value of

$$\int_0^{\infty} \Phi_1^T(E)\,\Phi_o^T(E)\frac{1}{E}\,e^{-\frac{E}{T}}\,dE \text{ is nearly } \left(\frac{2}{\sqrt{6\pi}}\right),$$

$$C = \frac{D_o^2}{6\lambda_1} \tag{50}$$

In table I, the time dependent eigenvalues for the free gas case are shown as unit of $\frac{M}{m}\frac{1}{\Sigma_f v_o}$ where the 20×20 matrices which remain the terms until the $L_{20}^{(1/2)}(x)$ are solved.

Table I shows that the ratios of $\lambda_{n+1}/\lambda_n (n > 1)$ in the case of mass 1 are smaller than the ratio in the case of heavy mass. This makes it difficult to distinguish the λ_1 from the higher eigenvalues in case of free-gas with mass 1. In the case of comparatively heavy gas like the one of mass 10, their eigenvalues approach those of the heavy gas model, but the high eigenvalues are different from those of the heavy gas. This means that, in this case, the heavy gas model is not applicable to the analysis in the high energy region.

Figure 1 shows the eigenfunctions of mass 1, 2, ∞, which are calculated from 10×10 dimensioned matrix.

The eigenvalues for mass 1, calculated from the several dimensioned matrices are shown in table II in order to see their convergence, and their eigenfunctions are shown in figure 2. The convergence appears comparatively slow, and the higher eigenfunctions show different shapes in the various matrix dimensions.

Next, the space dependent eigenvalues and eigenfunctions are shown in table III, and figure 4. Similarly to the time dependent case, the ratio of spatial eigenvalues B_{n+1}^2/B_n^2 decreases when the mass approaches to 1. The convergence of spatial eigenvalues in the case of mass 1 is shown in table IV. The convergence is faster than in the time dependent case. We can easily understand this fact, if we consider that the first order Laguerre polynomials are the spatial eigenfunctions in the heavy gas model.

3.1 — Heavy crystalline model

Next, we are going to consider the effect of the chemical binding on neutron thermalization by taking the heavy crystalline model, where the mass M is so heavy that the first power of $1/M$ is taken in the expansion of eq. (30). The time and spatial eigenvalues in the heavy crystalline model with the Debye frequency are shown with the thermalization power M_2 in table V.

The eigenvalues of graphite crystals in room temperature are calculated with the frequency which was Yoshimori and Kitano (19) calculated for the study of specific heat. In the case that graphite is assumed to be the heavy crystalline model the eigenvalues are shown in table IV, and their eigenfunction in figure 4.

In the case of simple energy independent diffusion coefficient, the formulation for the diffusion cooling coefficient is described in eq. (49). However, we should carefully compare the results obtained with experimental values by including the effect of energy dependent diffusion coefficient and the correction of the B^6 term. Thus we just have to compare the obtained results with the values calculated from the other theories, i.e. the values of $\overline{\lambda_1}$ in eq. (49), λ_1 in eq. (50) are compared with λ_{M2} in eq. (46).

If we assume that beryllium is the heavy crystalline material at the Debye temperature ($\theta = 1000°\mathrm{K}$), we get the value of $\lambda_1 M/\Sigma_B m v_o = 0.38$, $\overline{\lambda_1} M/\Sigma_B m v_o = 0.5020$. The latter value is smaller than the value calculated from eq. (46) $\lambda_{M2} M/\Sigma_B m v_o = 1.685$ by a factor 3.36, and approaches the old experimental value measured by Komoto and Kloverstom (1958) rather than the recent data measured by de Saussure and Silver (1958).

In the graphite which is assumed a heavy crystalline with the frequency function of the Yoshimori-Kitano model, $\lambda_1 M/\Sigma_B m v_o = 0.333$ and $\overline{\lambda_1} M/\Sigma_B m v_o = 0.399$ are obtained, and the value is smaller than the $\lambda_{M2} M/\Sigma_B m v_o = 0.957$ by a factor 2.4. According to the Krumhansl and Brooks (21) model whose frequency function is the Debye frequency with $\theta_z = 900°K$, $\theta_{xy} = 2500°\mathrm{K}$, the value of $\lambda_{M2} M/\Sigma_B m v_o$ is 0.843. These results show that high matrix elements are very important in the calculation of diffusion cooling coefficients.

Singwi calculated the effect of this non Maxwellian distribution for the diffusion cooling coefficient by taking the first three terms of the Laguerre expansion of the flux. However, by using the heavy gas model instead of heavy crystalline model, he estimated this value to be nearly 20 %. This is underestimated. If we take the 3×3 matrix which corresponds to the Singwi's correction, the values of $\lambda M/\Sigma_B m v_o$ beryllium and graphite are 1.172, 0.649 respectively, where λ is the time dependent first eigenvalue calculated from the 3×3 matrix.

mass	(1)	0	1	2	3	4	5	6	7	8	9
1	1.064	0	0.9242	1.131	1.300	1.531	1.806	2.110	2.436	2.777	3.132
2	1.638	0	1.318	1.699	2.107	2.635	3.235	3.881	4.560	5.265	5.992
3	1.954	0	1.541	2.130	2.761	3.563	4.467	5.438	6.457	7.517	8.611
4	2.153	0	1.685	2.478	3.306	4.356	5.539	6.812	8.154	9.554	11.01
5	2.289	0	1.786	2.764	3.769	5.043	6.480	8.034	9.680	11.40	13.20
10	2.608	0	2.03	3.643	5.318	7.414	9.826	12.49	15.38	18.47	21.75
∞	3.009	0	2.352	5.207	8.889	13.54	19.19	25.85	33.57	42.40	52.45

mass	10	11	12	13	14	15	16	17	18	19
1	3.499	3.879	4.271	4.679	5.103	5.549	6.023	6.536	7.110	7.800
2	6.741	7.512	8.309	9.133	9.992	10.89	11.85	12.88	14.04	15.42
3	9.739	10.90	12.10	13.34	14.64	16.00	17.44	18.99	20.73	22.82
4	12.51	14.05	15.66	17.32	19.05	20.86	22.79	24.87	27.28	30.00
5	15.06	16.99	18.99	21.06	23.22	25.50	27.91	30.52	33.43	36.94
10	25.21	28.87	32.70	36.73	40.97	45.45	50.23	55.42	61.28	68.38
∞	63.83	76.69	91.20	107.6	126.0	146.9	170.8	199.0	277.8	277.9

Table I

THE TIME DEPENDENT EIGENVALUES FOR THE FREE GAS

Unit is $\frac{1}{\Sigma_f v_n}\frac{M}{m}$. The values in column (1) are the matrix element S_{11}^{T}.

Dimension of matrix	1	2	3	4	5	6	7	8
17 × 17	0.9244	1.141	1.339	1.606	1.918	2.262	2.629	3.014
14 × 14	0.9246	1.158	1.396	1.711	2.075	2.474	2.900	3.350
11 × 11	0.9252	1.186	1.486	1.872	2.315	2.800	3.326	3.899
8 × 8	0.9273	1.243	1.647	2.156	2.744	3.417	4.231	—

Dimension of matrix	9	10	11	12	13	14	15	16
17 × 17	3.416	3.835	4.273	4.734	5.224	5.754	6.345	7.056
14 × 14	3.827	4.335	4.885	5.499	6.237	—	—	—
11 × 11	4.541	—	—	—	—	—	—	—

Table II

THE CONVERGENCE OF TIME DEPENDENT EIGENVALUES IN THE CASE OF MASS 1

(The values of $\frac{\lambda}{v_a}\frac{l}{\Sigma_f}$ are shown.)

mass \ i	0	1	2	3	4	5	6	7	8	9
1	0	0.3284	0.6201	0.9022	1.179	1.453	1.725	1.994	2.263	2.532
2	0	0.5259	1.077	1.621	2.159	2.693	3.223	3.751	4.277	4.802
3	0	0.6370	1.406	2.199	2.993	3.783	4.571	5.356	6.136	6.917
4	0	0.7068	1.646	2.661	3.698	4.740	5.781	6.821	7.859	8.894
5	0	0.7543	1.827	3.033	4.293	5.576	6.864	8.156	9.445	10.74
10	0	0.8646	2.301	4.116	6.182	8.413	10.75	13.17	15.63	18.12
∞	0	1	3	6	10	15	21	28	36	45

mass \ i	10	11	12	13	14	15	16	17	18	19
1	2.796	3.062	3.327	3.592	3.855	4.119	4.382	4.649	5.069	11.14
2	5.324	5.847	6.368	6.888	7.407	7.925	8.441	8.965	9.483	16.70
3	7.696	8.474	9.250	10.03	10.80	11.57	12.35	13.12	13.90	21.41
4	9.930	10.96	12.00	13.03	14.05	15.09	16.12	17.16	18.21	25.71
5	12.02	13.31	14.60	15.89	17.18	18.47	19.77	21.08	22.42	29.80
10	20.63	23.16	25.70	28.25	30.81	33.39	36.03	38.83	41.77	48.35
∞	55	66	78	81	95	110	126	143	161	180

Table III

THE SPACE DEPENDENT EIGENVALUES FOR THE FREE GAS

(where the product of *ith* spatial eigenvalue times $\frac{M}{m}\frac{1}{4\Sigma_t}(i+1)$ are shown in this table)

Dimension of matrix	8	9	10	11	12	13	14	15	16
17 × 17	2.263	2.530	2.796	3.062	3.327	3.593	3.859	4.191	8.785
14 × 14	2.263	2.530	2.797	3.064	3.349	6.624	—	—	—
11 × 11	2.263	2.532	4.672	—	—	—	—	—	—

Table IV

THE CONVERGENCE OF THE SPACE DEPENDENT EIGENVALUES IN THE FREE GAS OF MASS 1

The eigenvalues lower than 8th correspond to the results obtained from 20×20 matrix.

This table shows the products of the *ith* spatial eigenvalue times $\frac{M}{m} \frac{1}{4\Sigma_f} (i + 1)$

Debye temp. / Temp	S^{T}_{11}	i / $\frac{S_{11}}{S_{11}\ at\ =\ O}$	0	1	2	3	4	5	6	7
0	3.009	1	0	—	—	—	—	—	—	—
1	2.839	0.9434	0	1.906	4.636	9.446	16.33	25.75	38.70	57.80
2	2.412	0.8017	0	1.025	3.271	7.542	14.03	23.13	35.81	54.62
3	1.901	0.6317	0	0.5093	2.089	5.645	11.51	20.02	32.13	50.32
4	1.425	0.4734	0	0.2708	1.205	4.072	9.157	16.91	28.23	45.52
5	1.037	0.3445	0	0.1571	0.6931	2.810	7.164	14.12	24.53	40.77
6	0.7447	0.2475	0	0.09754	0.4187	1.865	5.544	11.69	21.18	36.27
7	0.5349	0.1778	0	0.06466	0.2744	1.251	4.267	9.684	18.29	32.25
8	0.3876	0.1288	0	0.04452	0.1892	0.8632	3.239	8.026	15.81	28.68
9	0.2849	0.0947	0	0.03172	0.1357	0.6177	2.439	6.658	13.70	25.55
Graphite Spectrum	0.9939	0.3303	0	0.3332	1.072	2.949	6.548	12.57	21.78	36.44

Table V

THE TIME DEPENDENT EIGENVALUES OF THE HEAVY DEBYE CRYSTALLINE MODEL AND THE GRAPHITE

(where the values of $\frac{M\lambda_i}{\Sigma_n m V_n}$ are shown)

Debye temp / Temp	S_n \ i	0	1	2	3	4	5	6	7
0	1	0	1	3	6	10	15	21	28
1	0.9434	0	0.9382	2.739	5.358	8.825	13.25	.18.79	25.69
2	0.8017	0	0.7492	1.996	3.906	6.782	10.79	16.10	23.07
3	0.6317	0	0.4985	1.270	2.717	5.162	8.775	13.77	20.65
4	0.1734	0	0.3003	0.7739	1.873	3.941	7.122	11.70	18.30
Graphite Spectrum	0.3303	0	0.2653	0.7496	1.582	3.049	5.416	9.020	14.55

Table VI

THE SPATIAL EIGENVALUES OF THE HEAVY DEBYE CRYSTALLINE MODEL AND THE GRAPHITE

(where the product of *ith* spatial eigenvalue times $\frac{M}{m}\frac{1}{4\Sigma_n}(i+1)$ are shown)

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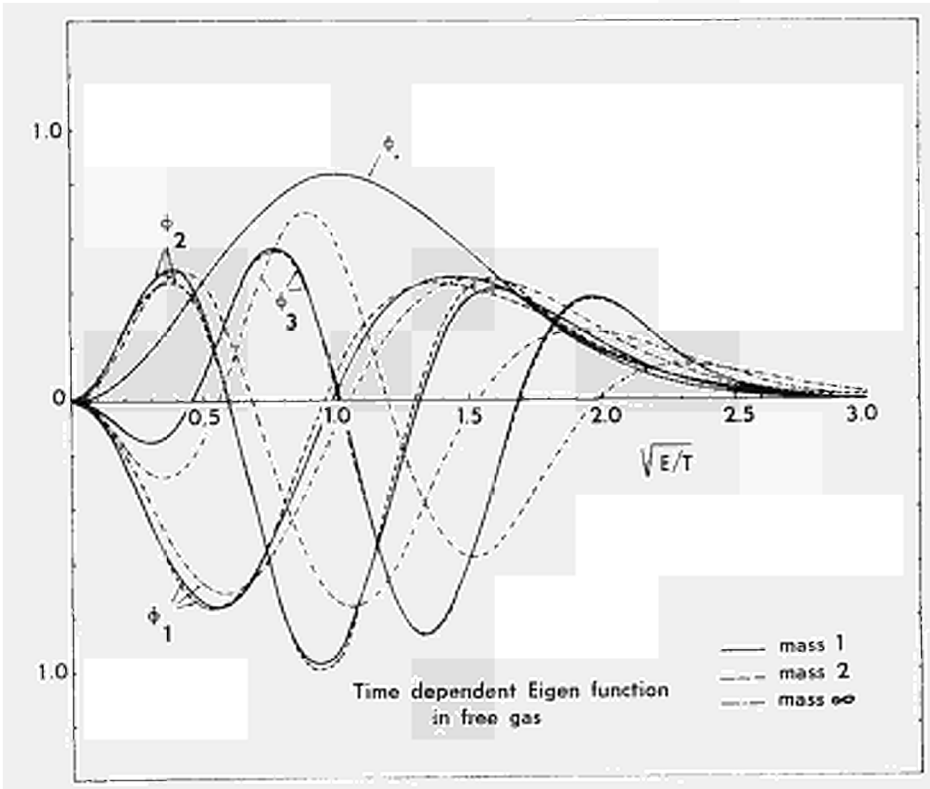
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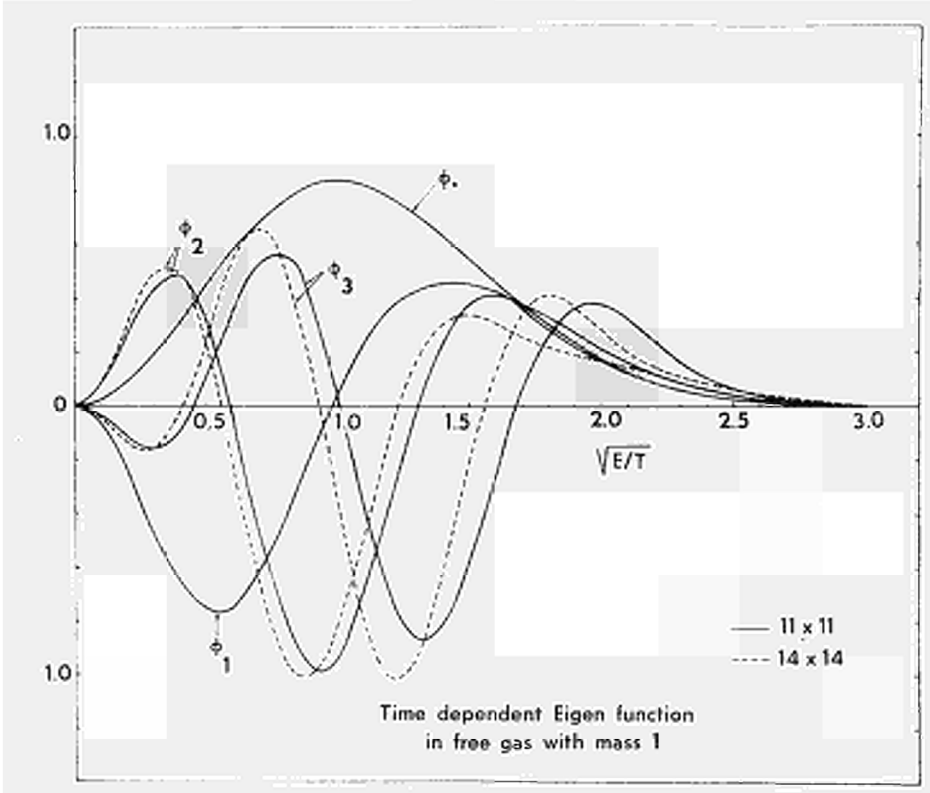
0.5
1.0
1.5
2.0
2.5
3.0
√E/T
Φ.
Φ2
Φ3
Φ1
mass 1
mass 2
mass ∞
Time dependent Eigen function
in free gas

FIG. 1.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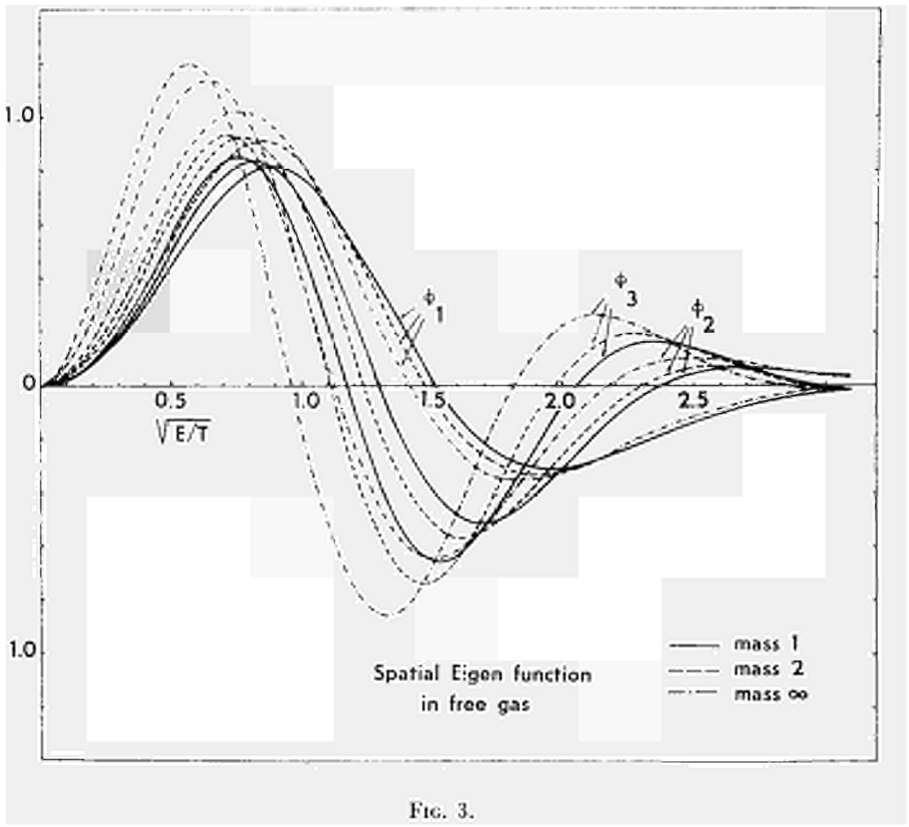
11 x 11
14 x 14
Time dependent Eigen function
in free gas with mass 1

FIG. 2.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√E/T
1.0
1.5
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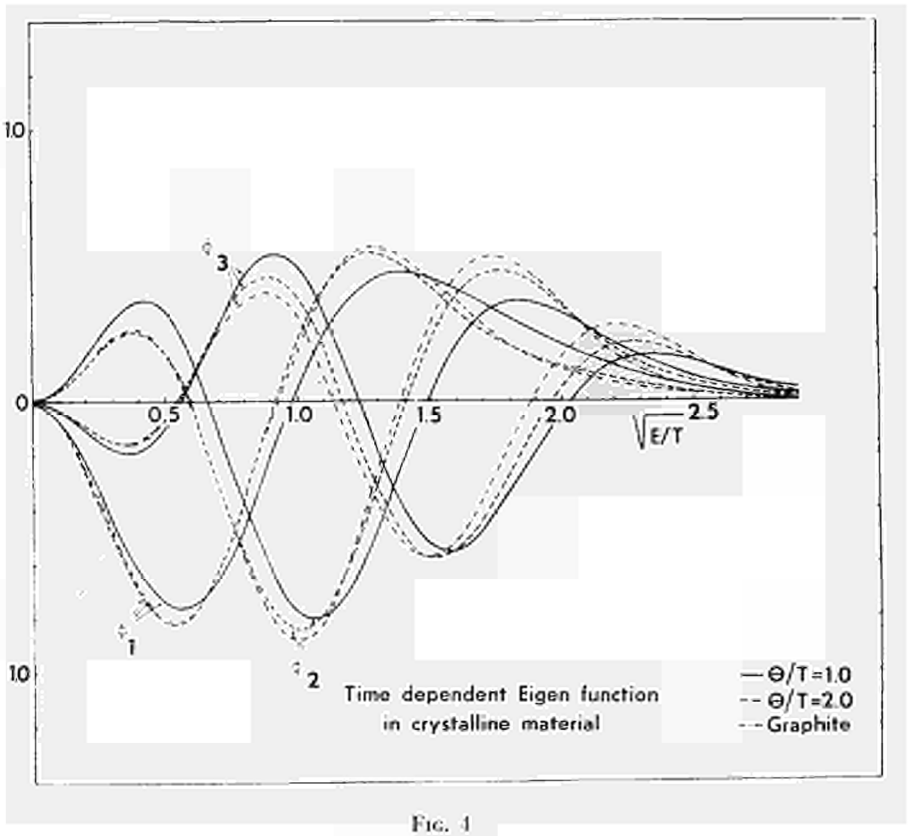
Φ1
Φ3
Φ2
Spatial Eigen function
in free gas
mass 1
mass 2
mass ∞

FIG. 3.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0
10
0.5
1.0
1.5
2.0
2.5
√E/T
Φ3
Φ1
Φ2
Time dependent Eigen function
in crystalline material
—Θ/T=1.0
--Θ/T=2.0
---Graphite

FIG. 4

CDNA00022ENC